Thermal conductivity across a twin boundary in d-wave superconductor

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We consider excitation spectrum near a twin boundary in an orthorhombic $d+s$ superconductor. The low-energy spectrum is highly sensitive to the presence of the small amount of s-wave component. Robustness of the bound states at the Fermi level with respect to impurities and an extra boundary potential is investigated. The role of Andreev transmission process for the low-temperature thermal conductivity across twin boundaries is studied for an impure superconductors. At very low temperatures the bulk part and the twin boundaries part of the thermal conductivity have similar linear-T dependences, whereas at intermediate temperatures the two contributions behave like T^3 and T^2, respectively.

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I. INTRODUCTION

The bound and extended quasiparticle states at twin boundaries in an orthorhombically twinned d-wave superconductor (like, supposedly, $YBa_2Cu_3O_{7-x}$) have recently been studied for the clean case.[1] An areal density of low energy twin-boundary bound states proportional to the magnitude of the s-wave component of the superconducting gap (which is a linear combination of tetragonal s-wave and d-wave components[2,3]) was found, and a process of Andreev transmission (particle-hole conversion in transmission across the twin boundary) was shown to be the essential mechanism of transporting heat across the twin boundaries in the limit of sufficiently low temperatures.

The present article considers the effect of disorder on the twin-boundary bound and extended states. A number of studies have shown the presence of impurities gives rise to a significant bulk density of zero energy excitations in the d-wave superconductor and that these have a significant effect on the bulk thermal conductivity.[4,5,6,7,8,9,10,11] This paper shows that the enhanced density of states at the Fermi level affects also the transport of heat across the twin boundaries. Furthermore, in addition to giving a finite lifetime to the extended bulk excitations, impurities transform the twin-boundary bound states into decaying resonances.

Theoretical calculations (see, e.g., Ref. 7) show that for a d-wave superconductor the low temperature a–b plane penetration depth varies linearly with T in the clean limit, but that impurity scattering can change this variation to T^2. Since this result depends essentially on the fact that the gap displays lines of nodes, and not on the d-wave symmetry, it is applicable to $YBa_2Cu_3O_{7-x}$ (YBCO), where the orthorhombic A_{1g} gap is considered to be a mixture of s-wave and d-wave components. In the Born limit, the amount of scattering required to produce the T^2 variations of the penetration depth is so large that T_c will be dramatically reduced, but in the unitary limit impurity scattering can give the T^2 temperature dependence without greatly affecting T_c. Very clean superconductors do show[12] the low temperature a–b plane penetration depth varying linearly with T whereas detailed analysis[13,14] of the results from a number of other samples reveals a T^2-behavior. For these reasons, much recent work has analyzed the effect of the unitary-limit impurity scattering on the properties of high-temperature superconductors.

Since a somewhat intuitive approach will be used below for calculation the thermal conductivity of the twin boundaries (e.g., in comparison with the Ambegaokar-Griffin[15] approach to the calculations of bulk thermal conductivity), we review here the relevant qualitative ideas and their application to the description of other properties of high-temperature superconductivity. For a clean d-wave superconductor the density of states for the excitations in the superconducting state varies linearly with excitation energy at low energies and can be written in the form

$$N_s(E)/N_0 \simeq E/\Delta_0 \ , \tag{1}$$

where N_0 is the normal state density of states and Δ_0 is the maximum gap. In the strong scattering limit, the energy of low-lying excitations with wave-vector $\mathbf{k}$ acquires an imaginary part, i.e., $E_{\mathbf{k}}$ becomes $E_{\mathbf{k}} + i\Gamma$, thus the excitation possessing a lifetime $\tau = 1/(2\Gamma)$ ($\hbar = 1$). The quantity Γ is given by the solution of the following equation (see, e.g., Ref. 8)

$$\Gamma^2 = \frac{n_i \Delta_0}{2N_0 \ln(4\Delta_0/\Gamma)} \ , \tag{2}$$

where n_i is the impurity concentration. Note that this result for the damping of an excitation is independent of the wave-vector and energy, and is valid for quasiparticles with energies less than Γ. Since, by the uncertainty principle, the low-energy excitations will have a spread in energy of the order of Γ, excitations with $E_{\mathbf{k}}$ from zero

up to Γ should contribute to the density of states at zero energy. Thus, taking account of Eq. (1), we have

$$N_s(E)/N_0 \simeq \Gamma/\Delta_0 \tag{3}$$

for the density of superconducting excitations at zero energy in the presence of unitary-limit impurity scattering. The exact result[8] differs from this by a logarithmic factor which varies weakly with impurity concentration and which is often neglected in qualitative discussions.[6] The low temperature specific heat associated with this constant density of states at low energies is ($k_B = 1$)

$$C_V = \frac{2\pi^2}{3} N_0 \frac{\Gamma}{\Delta_0} T \ . \tag{4}$$

These ideas allow an estimate of the bulk thermal conductivity to be made as[10]

$$\kappa \sim C_V v_F l \sim \left(N_0 \frac{\Gamma}{\Delta_0} T \right) v_F \left(v_F \frac{1}{\Gamma} \right) = \frac{\pi^2}{3} \frac{v_F^2 N_0}{\Delta_0} T \ . \tag{5}$$

Note that, like the result for the electrical conductivity in the unitary limit of impurity scattering,[6] this is a universal result. The parameter Γ, which depends on n_i, cancels out and the thermal conductivity is independent of the impurity concentration and the strength of impurity potential. Recently, the universal heat transport has been observed[16] in untwinned crystals $YBa_2(Cu_{1-x}Zn_x)_3O_{6.9}$. Quantitative comparison of these data with the theory suggests that quasiparticle scattering on Zn impurities in YBCO is close, but does not coincide completely with the unitary limit.

At higher energies $\Gamma \ll E \ll \Delta_0$ the density of states reverts to it's clean-limit value (1), whereas the relaxation rate of superconducting quasiparticles acquires energy dependence $\Gamma_S = \Gamma_N \Delta_0/E$ (Ref. 6), where the normal state relaxation rate in the unitary limit is $\Gamma_N = n_i/\pi N_0$. In the corresponding temperature range $\Gamma \ll T \ll \Delta_0$ the electronic thermal conductivity can be calculated by an elementary Boltzman equation approach[17]

$$\kappa = \sum_{\mathbf{k}} \frac{(E_{\mathbf{k}} v_{\mathbf{k}} \cos\theta_{\mathbf{k}})^2}{T\Gamma_S} \left(-\frac{\partial f_{\mathbf{k}}^0}{\partial E_{\mathbf{k}}} \right) . \tag{6}$$

provided the correct energy dependence of Γ_S given above is taken into account. Using the fact that near the gap nodes the quasiparticle group velocity reduces to v_F, we find after integration

$$\kappa = \frac{7\pi^4}{15} \frac{v_F^2 N_0}{\Gamma_N \Delta_0^2} T^3 \ . \tag{7}$$

Thus, above the universal linear-T behavior at very low temperatures the heat current in d-wave superconductor varies as T^3, which is consistent with the numerical data presented in Ref. 10.

II. QUASIPARTICLE STATES NEAR TWIN BOUNDARY

In a tight-binding model on a square lattice (supposedly reproducing in a more or less correct fashion a single CuO_2 plane in YBCO), the Green function describing the excitations in the superconducting state is determined by the equation

$$\sum_k \left[\hat{1}\tilde{z}\delta_{ik} - \hat{\epsilon}_{ik} \right] \hat{G}(k,j,z) = \hat{1}\delta_{ij} \ . \tag{8}$$

Singlet state pairing is assumed and a "hat" indicates a 2×2 matrix in particle-hole space. Disorder is included in this model by considering impurities on randomly chosen lattice sites, each impurity being described by an additional potential u. Impurity scattering is treated in the self-consistent t-matrix approximation. As a result, the quantity $\tilde{z}$ must be determined from the equation

$$\tilde{z} = z - \frac{n_i u^2 \mathcal{G}_0(\tilde{z})}{1 - u^2 \mathcal{G}_0(\tilde{z})^2} \ , \tag{9}$$

where

$$\mathcal{G}_0(\tilde{z}) = \tfrac{1}{2} \mathrm{Tr} \hat{G}(i,i,z) \ . \tag{10}$$

The right hand side of Eq. (10) is assumed to be independent of site index i, z is the usual Matsubara frequency, and the s-wave component of the gap is assumed negligible in comparison with the d-wave component in arriving at Eq. (9).

In the unitary limit ($u \to \infty$) detailed study of Eq. (9) shows that for low energy excitations, i.e., excitations having an energy less than Γ, the quantity $\tilde{z}$ is given by

$$\tilde{z} = z \pm i\Gamma \tag{11}$$

where Γ has been defined in the Introduction, and the upper and the lower signs refer to the upper and lower half plane, respectively.

The matrix $\hat{\epsilon}_{ik}$ contains the same quantities that were used in our previous model of a clean superconductor containing a twin boundary:[1]

$$\hat{\epsilon}_{ik} = \hat{\tau}_3 \left(-t_{ik} - \mu\delta_{ik} + U_0 \delta_{ik} \delta_{i\mathrm{B}} \right) + \hat{\tau}_1 \Delta_{ik} \tag{12}$$

where $\delta_{i\mathrm{B}}$ is unity for i on the twin boundary and zero otherwise and Δ_{ik} is assumed real.

When the site indices are incorporated into the matrix notation, Eq. (8) becomes

$$\left[\hat{1}\tilde{z} - \hat{\epsilon} \right] \hat{G} = \hat{1} \ . \tag{13}$$

where $\tilde{z}$ is given by Eq. (11). Since $\hat{\epsilon}$ is a real symmetric matrix, it can be diagonalized by a unitary transformation, say S, giving

$$\hat{G} = S^\dagger (\hat{1}\tilde{z} - \hat{\Lambda})^{-1} S \ , \tag{14}$$

where $\hat{\Lambda}$ is the diagonal matrix of the eigenvalues of $\hat{\epsilon}$. The excitation energies are found from the poles of $\hat{G}$ when $z \to E + i0$. Thus, in the low-energy limit, if Λ_i is an eigenvalue of ϵ, there will be an excitation with energy

$$E = \Lambda_i + i\Gamma \ . \tag{15}$$

Therefore, all low energy excitations, including those which would be bound to the surface in the absence of impurity scattering, will have the same lifetime $\tau = 1/2\Gamma$.

Diagonalization of the tight-binding Hamiltonian

The diagonalization of $\hat{\epsilon}$ is essentially the same as in Ref. 1. Here we give some details not previously explicitly described, and in particular calculate transmission coefficients across the twin boundary in the superconducting state.

We do not solve the problem for the superconducting order parameter near the twin boundary self-consistently, but instead substitute a "guess" order parameter into the Bogoliubov-de Gennes (BdG) equations

$$E\psi_i = \hat{\epsilon}_{ik}\psi_k \tag{16}$$

to study the qualitative features of the excitation spectrum. Definitions of nearest-neighbor hopping and pairing amplitudes are given in Fig. 1. In accordance with the orthorhombic symmetry of CuO_2 planes in YBCO these amplitudes are different along a and b axes: $t_{1,2} = t(1 \pm \epsilon)$ and $\Delta_{1,2} = \Delta(1 \pm \delta)$.

In the bulk of each twin, quasiparticles are plane waves with excitation energy

$$E_{\mathbf{k}} = \sqrt{\varepsilon(\mathbf{k})^2 + \Delta(\mathbf{k})^2} \ , \tag{17}$$

where the normal state quasiparticle dispersion in the right (left) twin is given by

$$\varepsilon(\mathbf{k}) = -4t \cos\frac{k_x a}{\sqrt{2}} \cos\frac{k_y a}{\sqrt{2}} \mp 4t\epsilon \sin\frac{k_x a}{\sqrt{2}} \sin\frac{k_y a}{\sqrt{2}} - \mu \ , \tag{18}$$

and the mixed symmetry superconducting gap is

$$\Delta(\mathbf{k}) = 2\Delta \sin\frac{k_x a}{\sqrt{2}} \sin\frac{k_y a}{\sqrt{2}} \mp 2\Delta\delta \cos\frac{k_x a}{\sqrt{2}} \cos\frac{k_y a}{\sqrt{2}} \ , \tag{19}$$

where the first term corresponds to a d-wave component, while the second term describes an extended s-wave component (the only s-wave harmonic in our model) which admixes with different signs in the two crystal twins. At half-filling the maximum amplitudes of the two harmonics are $\Delta_d = \Delta$ and $\Delta_s = \Delta\delta < \Delta_d$.

Treating quasiparticle scattering in both the normal and the superconducting states one can employ the translational invariance along the twin boundary, which leads to conservation of the parallel component of the momentum. For low-energy elastic processes we need to determine change in the normal component of the momentum of a scattered excitation. From (18), the normal components of the Fermi momenta for incoming and outgoing electrons with a given parallel component k_y are $k^{>}_{\pm x} = \pm k + q$, in the right twin, and $k^{<}_{\pm x} = \pm k - q$, in the left twin (see Fig. 2). Parameters k and q are defined by

$$\tan\frac{qa}{\sqrt{2}} = \epsilon \tan\frac{k_y a}{\sqrt{2}} \ , \qquad \cos\frac{ka}{\sqrt{2}} = \frac{-\mu\cos(qa/\sqrt{2})}{4t\cos(k_y a/\sqrt{2})} \ . \tag{20}$$

The normal components of the Fermi velocities for all these states have the same absolute value $v_{Fx} = 2\sqrt{2}ta\sin(ka/\sqrt{2})\cos(k_y a/\sqrt{2})/\cos(qa/\sqrt{2})$.

The two-component BdG eigenfunctions on the left and right sides, $\psi_i^{<}$ $(x<0)$ and $\psi_i^{>}$ $(x>0)$ in the twin boundary problem, are still given by a combinations of plane waves, therefore among BdG equations (16) a special care is required only for those with i on the twin boundary. Subtracting from the difference equation (16) for $i \in$ TB a uniform part and making Fourier transform over y we obtain two conditions: (i) continuity equation $\psi_0^{<} = \psi_0^{>}$ and (ii) an additional equation "on the derivative," which in the leading order in in superconducting gap, i.e., neglecting corrections $O(\Delta^2/\varepsilon_F)$ to the energy, has the following form

$$\psi_1^{>} e^{-iqa/\sqrt{2}} - \psi_1^{<} e^{iqa/\sqrt{2}} = \frac{U_0\cos(qa/\sqrt{2})}{2t\cos(k_y a/\sqrt{2})}\,\psi_0 \ . \tag{21}$$

In the following analysis we will also use the symmetry of the twin boundary which is expressed by the relations $t_{\hat{\sigma}i\hat{\sigma}j} = t_{ij}$ and $\Delta_{\hat{\sigma}i\hat{\sigma}j} = -\Delta_{ij}$, where $\hat{\sigma}$ is reflection in the twinning plane (not a Pauli matrix). The BdG equations (16) are invariant under the combined transformation $\hat{U} = \tau_3\hat{\sigma}$, τ_3 being the Pauli matrix which acts in the particle-hole space. All solutions are, hence, classified by their parity with respect to $\hat{U}$.

In the normal state, quasiparticles move freely across the twin boundary for $U_0 = 0$ and acquire a finite scattering amplitude $r = \alpha/(i-\alpha)$ for $U_0 > 0$.

Let us consider a scattering process below T_c during which a quasiparticle approaching the twin boundary from the right with the wave-vector $\mathbf{k}^{>}_{-}$ is reflected into an out-going state with the wave-vector $\mathbf{k}^{>}_{+}$ on the same side and is transmitted into out-going states with $\mathbf{k}^{<}_{-}$ and $\mathbf{k}^{<}_{+}$ on the left side (Fig. 2). We define $\Delta_- = \Delta(\mathbf{k}^{>}_{-})$, $\Delta_+ = \Delta(\mathbf{k}^{>}_{+})$, $\Delta(\mathbf{k}^{<}_{-}) = -\Delta_+$, and $\Delta(\mathbf{k}^{<}_{+}) = -\Delta_-$, the last two relations following from the symmetry of the superconducting state on the twin boundary.[3]

There are three cases for the quasiparticle energy E to be considered, (i) $E < \Delta_{\min}$, (ii) $\Delta_{\min} < E < \Delta_{\max}$, and (iii) $\Delta_{\max} < E$, where $\Delta_{\min} = \min(|\Delta_-|, |\Delta_+|)$ and $\Delta_{\max} = \max(|\Delta_-|, |\Delta_+|)$.

1. Bound states, $E < \Delta_{\min}$

The bulk states in this energy range are absent and the only possibility is states localized in the vicinity of the twin boundary. The wave function of a bound state in the right twin is given by

$$\psi_i^{>} = \begin{pmatrix} \Delta_- \\ E + i\Omega_- \end{pmatrix} e^{i\mathbf{k}_-^{>}\cdot\mathbf{r}_i - \kappa_- x} + R \begin{pmatrix} \Delta_+ \\ E - i\Omega_+ \end{pmatrix} e^{i\mathbf{k}_+^{>}\cdot\mathbf{r}_i - \kappa_+ x}$$

$$\Omega_\pm = \sqrt{\Delta_\pm^2 - E^2} \ , \quad \kappa_\pm = \Omega_\pm / v_{Fx} \tag{22}$$

whereas on the left side $\psi_i^{<}$ is obtained from $\psi_i^{<} = \pm\tau_3 \psi_{\hat{\sigma}i}^{>}$ for even (odd) eigenstates of the operator $\hat{U}$. The ratio of the particle-hole components of the wave-function is determined from homogeneous BdG equations, while energy E and "reflection" coefficient R have to be found from the continuity condition and Eq. (21). Let us consider these equations in more detail for the odd symmetry solutions. From the continuity of the wave function one finds

$$\Delta_- + R\Delta_+ = 0 \ , \tag{23}$$

whereas Eq. (21) yields

$$E + i\Omega_- - R(E - i\Omega_+) = i\alpha[E + i\Omega_- + R(E - i\Omega_+)] \ , \tag{24}$$

where $\alpha = U_0 a/\sqrt{2} v_{Fx}$. From the real part of the last equation we find for the bound state energy

$$E = \pm \frac{2\alpha|\Delta_-|}{\sqrt{4\alpha^2 + [1 - R - \alpha^2(1+R)]^2}} \ . \tag{25}$$

The sign in this equation should be found by substituting expression (25) back into Eq. (24). This gives

$$|1 - R - \alpha^2(1+R)| = \mp[1 - R - \alpha^2(1+R)] \tag{26}$$

and

$$\frac{R}{|R|} = \pm \frac{[\alpha^2(1+R) + 1 - R]}{|\alpha^2(1+R) + 1 - R|} \ . \tag{27}$$

As follows from Eqs. (26) and (27) the two cases $|R| < 1$ and $|R| > 1$ transform into each other under $R \leftrightarrow 1/R$. Consequently, we have to consider only $-1 < R < 1$.

For $-1 < R < 0$ or $\Delta_+\Delta_- > 0$ we find from Eq. (26) the upper sign if $\alpha^2 > (1-R)/(1+R)$ and the lower sign in the opposite case. On the other hand Eq. (27) gives always the lower sign. Therefore, the energies of the bound states of odd symmetry are given by (25) with the minus sign as far as the boundary potential is weak and α is small. The dispersion of bound state energies disappears at $U_0 = 0$. The condition $\Delta_+\Delta_- > 0$ is satisfied in the vicinity of the gap nodes, e.g., for $k_{y\mathrm{C}} < k_y < k_{y\mathrm{A}}$ and for $k_y > k_{y\mathrm{D}}$ and $k_y < k_{y\mathrm{B}}$ in Fig. 2. The number of the bound states is, thus, proportional to the degree of the orthorhombicity of the superconducting gap or Δ_s/Δ_d, where Δ_s and Δ_d are amplitudes of s- and d-wave gaps.[1] Observation of the zero-energy peak in the local density of states near twin boundary would be a direct experimental evidence of the mixed symmetry gap in YBCO.

The critical value of the boundary potential U_0, which destroys the bound states, is different for states propagating normally to the twinning plane and for states propagating nearly parallel. In the former case $\alpha \sim U_0/\tilde{\varepsilon}$, where $\tilde{\varepsilon}$ is geometrical average of the Fermi energy ε_F and the band width. The parameter α is, therefore, quite small and cannot exceed the critical value $\alpha_c = 1$. The bound states lie near the Fermi level having a weak dispersion given by Eq. (25). In the second case of the bound states with momenta nearly parallel to the twin boundary, perpendicular component of the Fermi velocity is very small and α is significantly enhanced. Bound states near "vertical" nodes in Fig. 2 disappear completely for $U_0/\tilde{\varepsilon} > \Delta_s/\Delta_d$.

For $0 < R < 1$ or $\Delta_+\Delta_- < 0$, that is, in the "out of nodes" region, Eq. (27) yields the upper sign. This is compatible with Eq. (26) if $\alpha^2 > (1-R)/(1+R)$. Arbitrary weak boundary potential can produce bound states for the part of the Fermi surface with $R \approx 1$. Total number of such bound states is, however, proportional to α. As a substitution of $R \approx 1$ into (25) shows, these bound states split from the bottom of the continuum of bulk quasiparticles, i.e., have energies slightly below $\Delta(\mathbf{k})$, which does not vanish in this region of the Fermi surface. Therefore, such a possibility being sensitive to the value of the boundary potential is less important for the thermodynamic of the system.

Completely analogous consideration of the even symmetry states predicts the upper sign in Eq. (25) and the same condition on the two gaps

$$\Delta_+\Delta_- > 0 \tag{28}$$

in order to have bound quasiparticle states on the twin boundary.

Disorder provides an additional mechanism for broadening the zero-energy peak in the local density of states on twin boundary. The critical impurity concentration, which smears out completely bound states, is obtained by the following arguments. The characteristic space extension of bound states is $\xi_s = v_F/\pi\Delta_s$. In the clean limit they can be considered as quasiparticles undergoing multiple Andreev reflections in the superconducting well on the twin boundary. In the presence of impurity scattering, the coherence length ξ_s has to be compared to the mean free path $l = v_F\tau = v_F/2\Gamma$. For $\xi_s \ll l$, a quasiparticle is reflected many times before being wiped out from the twin boundary region by a scattering on an impurity. In this case, though being transformed into resonances, the quasibound states are still well defined. For $\xi_s \geq l$, a quasiparticle scatters to the continuum very quickly and the twin boundary resonances as well as the zero-energy peak disappear. Thus, it is possible to destroy the zero-energy peak in the local density of states

by increasing number of impurities to the critical value given by $\Gamma_c \sim \Delta_s$.

2. Extended states with $|\Delta_-| < E < |\Delta_+|$

In this energy range, an excitation, particle or hole, can approach the twin boundary from the bulk, but it cannot be reflected back into the twin with the wave-vector $\mathbf{k}_+^>$, since $E < |\Delta_+|$. The only allowed processes are Andreev reflection[18] and Andreev transmission,[1] which involve particle-hole transformations. The wave function of such a quasiparticle is given for $x > 0$ by

$$\psi^> = \begin{pmatrix} \Delta_- \\ E_- \end{pmatrix} e^{i\mathbf{k}_-^> \cdot \mathbf{r}} + A \begin{pmatrix} E_- \\ \Delta_- \end{pmatrix} e^{i\mathbf{k}_-^> \cdot \mathbf{r}} + B \begin{pmatrix} \Delta_+ \\ E_+ \end{pmatrix} e^{i\mathbf{k}_+^> \cdot \mathbf{r} - \kappa_+ x}$$

and for $x < 0$

$$\psi^< = A' \begin{pmatrix} -\Delta_+ \\ E_+ \end{pmatrix} e^{i\mathbf{k}_-^< \cdot \mathbf{r} + \kappa_+ x} + B' \begin{pmatrix} E_- \\ -\Delta_- \end{pmatrix} e^{i\mathbf{k}_+^< \cdot \mathbf{r}} \ . \quad (29)$$

We have neglected in the above formulas small shifts of the wave vectors from the Fermi surface for propagating states and defined

$$E_- = E - \sqrt{E^2 - \Delta_-^2} \ , \quad E_+ = E - i\sqrt{\Delta_+^2 - E^2} \ . \quad (30)$$

Eqs. (29) describe an incident electron-like quasiparticle with momentum $\mathbf{k} \approx \mathbf{k}_-^>$ approaching the twin boundary from the right, a reflected hole with wave vector $\mathbf{k} \approx \mathbf{k}_-^>$ and transmitted hole with $\mathbf{k} \approx \mathbf{k}_+^<$. There are also two damped waves with wave vectors $\mathbf{k}_+^>$ and $\mathbf{k}_-^<$. We also took into account the odd symmetry of the gap with respect to the reflections in the twinning plane.

Parameters A, A', B, and B' have to be determined from the continuity of the wave function and Eq. (21). For zero boundary potential one finds $B = B' = 0$ so that only exponentially decaying wave exists for $x < 0$. Hence, the transmission coefficient through the twin boundary for quasiparticles with $|\Delta_-| < E < |\Delta_+|$ vanishes.

For $U_0 \neq 0$ there is a nonzero probability of an incident electron at $\mathbf{k}_-^>$ to be transformed into an outgoing hole of wave-vector $\mathbf{k}_+^<$ on the opposite side of the boundary, which is a kind of Andreev transmission. Remarkably, the boundary barrier $U_0 > 0$, which causes reflection of the quasiparticles from the twin boundary in the normal state, allows transmission of the low-energy excitations in the superconducting state. The particle-hole transmission coefficient to the second order in a small parameter α is

$$w_{\text{ph}} = |B'|^2 = w_0 \frac{\Delta_+^4 (E_-^2 - \Delta_-^2)^2}{|\Delta_- \Delta_+ + E_- E_+|^4} \ , \quad (31)$$

where $w_0 = 4\alpha^2 = 2(U_0 a / v_F)^2$. For $E \ll \Delta_+$ the transmission coefficient simplifies to

$$w_{\text{ph}} \approx w_0 (E^2 - \Delta_-^2)/E^2 \ . \quad (32)$$

3. Extended states with $E > \Delta_{\max}$

The wave function of scattered quasiparticle on the left and right sides is given by the same expression (29) except for the decaying factors $e^{\pm\kappa_+ x}$, which are absent now, and E_+ defined as $E_+ = E - (E^2 - \Delta_+^2)^{1/2}$ instead of Eq. (30). The outgoing quasiparticle flow on the left side consists now of two parts corresponding to electron and hole excitations. Therefore, the transmission coefficient has the particle-hole contribution w_{ph} of Eq. (31) and the particle-particle contribution

$$w_{\text{pp}} = |A'|^2 \frac{\Delta_+^2 - E_+^2}{\Delta_-^2 - E_-^2} = \frac{(\Delta_+^2 - E_+^2)(\Delta_-^2 - E_-^2)}{(\Delta_- \Delta_+ + E_- E_+)^2} \ , \quad (33)$$

where the second equality is obtained for $\alpha \ll 1$. For high energies $E \gg \Delta_{\max}$ in this case the particle-particle transmission coefficient $w_{\text{pp}} \approx 1$ and $w_{\text{ph}} = O(\alpha^2)$.

III. THERMAL RESISTANCE OF TWIN BOUNDARY

In the case of dirty superconductor with strong impurity scatters, the width Γ of the low-lying energy levels has an important implication on the thermal conductivity through the twin boundaries. For $\Gamma > \Delta_s$, excitations with energies approximately equal to Γ will be the most important carriers of heat at low temperatures, completely analogous to the case of the bulk thermal conductivity (see Introduction). For these excitations $w \approx 1$ (if $\alpha \ll 1$) and the flow of the heat will not be much affected by the presence of the twin boundaries even in the low-temperature limit.

For $\Gamma < \Delta_s$, the situation is different. At low temperatures ($T \ll \Gamma$) the heat will again be carried primarily by excitations with energies $E \approx \Gamma$ and the mechanism of the Andreev transmission discussed above produces a nonzero flow of heat across the twin boundary. Following Andreev,[18] the heat current across the boundary is given by the expression

$$W = \frac{2}{L^3} {\sum_{\mathbf{k}}}' E_{\mathbf{k}} n_{\mathbf{k}} v_{kx} w_{\mathbf{k}} \ . \quad (34)$$

Here, the prime attached to the sum over momenta means that only excitations with x component of the group velocity satisfying $v_{kx} < 0$ are summed over; the x-axis is the axis normal to the twin boundary. Also, excitations with wave vectors near $\mathbf{k}_{\text{B}}$ and $\mathbf{k}_{\text{D}}$ in Fig. 2 are neglected since their group velocities toward the twin boundary are small. The factor 2 accounts for the contribution of two spin directions.

For excitations near $\mathbf{k}_{\text{A}}$ and $\mathbf{k}_{\text{C}}$ (Fig. 2), the normal projection of the group velocity is

$$v_{kx} = v_F \sqrt{E_{\mathbf{k}}^2 - \Delta_{\mathbf{k}}^2} / E_{\mathbf{k}} \ . \quad (35)$$

Thus, using Eq. (32) for the transmission coefficient we have

$$v_{kx}w_{\mathbf{k}} = v_F w_0 \left(\frac{\sqrt{E_{\mathbf{k}}^2 - \Delta_{\mathbf{k}}^2}}{E_{\mathbf{k}}} \right)^3 . \tag{36}$$

In integrating over $\mathbf{k}$ [on the right hand side of Eq. (34)] in the neighborhood of $\mathbf{k}_{\rm A}$ we approximate

$$E_{\mathbf{k}}^2 = (v_F \delta k_x)^2 + (v_\Delta \delta k_y)^2 \ , \qquad \Delta_{\mathbf{k}} = v_\Delta \delta k_y \tag{37}$$

and $|v_\Delta| \sim \Delta_0/k_F \ll v_F$. It is easily seen that the effect of the factor in brackets in Eq. (36), when averaged over k as in Eq. (34), is to give a factor of the order of unity. For example, if the exponent of the factor in square brackets were 2 rather than 3, evaluation of the sum over k in Eq. (34) shows that the correct result could be obtained by the substitution $v_{kx}w_{\mathbf{k}} = \frac{1}{2}v_F w_0$ for Eq.(36). Since the exponent is 3 not 2, we make a replacement

$$v_{kx}w_{\mathbf{k}} = f v_F w_0 \ , \tag{38}$$

where f will be close to, but somewhat less than unity. Impurity scattering could not change this factor by very much. With this substitution and extending the sum over k in Eq. (34) to all k, we find

$$W = \tfrac{1}{4} f v_F w_0 \left(\frac{2}{L^3} \sum_{\mathbf{k}} E_{\mathbf{k}} n_{\mathbf{k}} \right). \tag{39}$$

Note, that the quantity in the bracket is $\bar{E} - \mu N$, where $\bar{E}$ is the mean energy of the system.

If the temperature on both sides of the twin boundary is the same, the heat current W is balanced by a heat current of the same magnitude in the opposite direction. Thus, in the presence of a temperature difference across the twin boundary, there will be a net heat current given by

$$Q = \frac{\partial W}{\partial T}\delta T = \kappa_{\rm TB}\frac{\delta T}{d} \ , \tag{40}$$

where d is an average spacing between twin boundaries. Hence, the thermal conductivity, if limited by twin boundary resistance, will have the low-temperature form

$$\kappa_{\rm TB} = \tfrac{1}{2} C_V v_F \lambda_{\rm eff} \ , \tag{41}$$

where

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_{V,N} \approx \frac{\partial}{\partial T}(\bar{E} - \mu N) \tag{42}$$

and an effective mean free path

$$\lambda_{\rm eff} = \frac{f}{2} w_0 d \tag{43}$$

has been defined. In writing Eq. (42), a weak temperature dependence of the chemical potential has been neglected.

Note, that since v_F and $\lambda_{\rm eff}$ do not depend on T, the temperature dependence of the twin boundary thermal conductivity will be that of the specific heat.

In the unitary limit for impurity scattering, the low-temperature specific heat at $T < \Gamma$, has the form (4). Thus, the thermal conductivity due to the twin boundaries has the same linear-T dependence at low temperatures as the bulk thermal conductivity $\kappa_{\rm bulk}$. If we now consider a sample with one predominant orientation of twin boundaries, say parallel to (110), then the thermal resistance in the perpendicular direction is additive and for the combined thermal conductivity from boundaries and impurities we have

$$\kappa_\perp^{-1} = (\kappa_{\rm TB})^{-1} + (\kappa_{\rm bulk})^{-1} \ . \tag{44}$$

The heat flow in the parallel direction is unaffected by twin boundaries and $\kappa_\parallel = \kappa_{\rm bulk}$. Such anisotropy of in-plane thermal conductivity disappears for samples with equal weights of two types of twins.

For $\Gamma \ll T \ll \Delta_s$, the specific heat coincides with that of a clean d-wave superconductor $C_V = 9\zeta(3)N_0T^2/\Delta_0$. Thus both in this case and in the case $T > \Delta_s$, when the scattering can be treated in the Born approximation, the twin boundary thermal conductivity varies as T^2. For the sake of comparison we note that in the unitary scattering limit and $\Gamma \ll T \ll \Delta_0$ the bulk thermal conductivity varies as T^3 (see Introduction), whereas in the Born limit[11] and for $T \ll \Delta_0$, $\kappa_{\rm bulk}$ varies as T.

IV. CONCLUSIONS

In the previous work[1] on a clean $d + s$ orthorhombic superconductor, such as YBCO, we have demonstrated the existence of bound zero-energy excitations at the twin boundaries and identified an Andreev transmission process responsible for heat conduction across the twin boundaries at low temperatures. When strong impurity scatters are added, a new energy scale Γ appears, which is the relaxation rate of the lowest energy quasiparticles. In this paper we show that the twin boundary bound states remain well-defined resonances contributing a zero-energy peak to the local density of states at the twin boundary provided $\Gamma < \Delta_s$, where Δ_s is an amplitude of the s-wave component of the gap. Furthermore, we calculate the transmission coefficient describing the transmission of excitations across the twin boundaries, and hence evaluate the thermal conductivity of twin boundaries. For $\Gamma > \Delta_s$, the twin boundaries present resistance for the flow of heat due to an extra boundary potential only, i.e., the same as in the normal state. For $\Gamma < \Delta_s$, on the other hand, there are two cases to be considered. If $T \ll \Gamma$, the twin boundary thermal conductivity, like the bulk thermal conductivity, varies linearly with T, while if $\Gamma \ll T \ll \Delta_s$ (or if the impurity scatters are weak), the twin boundary thermal conductivity varies as T^2. The best way to identify twin boundary thermal conductivity

experimentally would be on a highly twinned sample with all twin boundaries parallel to the (110) plane; measurements of thermal conductivities in the [110] and the [$1\bar{1}0$] directions will then differ due to the thermal resistance of the twinning planes. Anisotropy in the basal plane thermal conductivity, which develops only below T_c, would be a clear indication of the particle-hole transformation in heat flow across twin boundaries.

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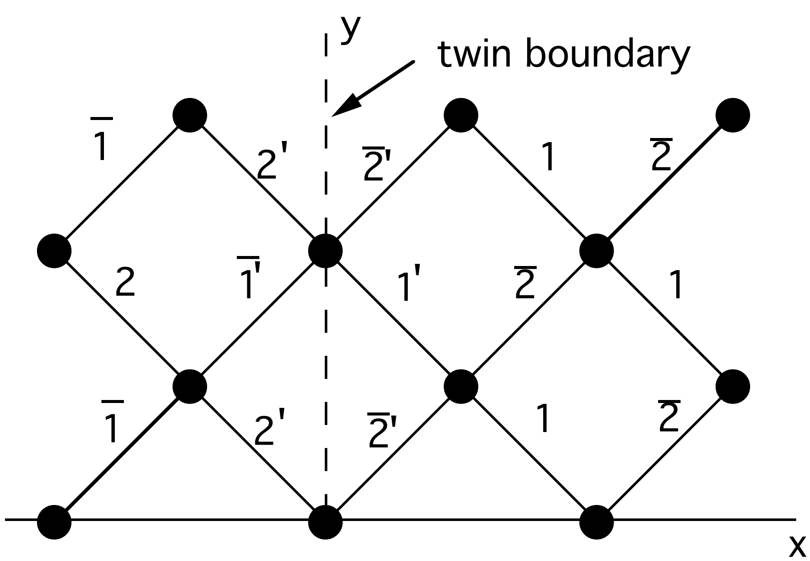
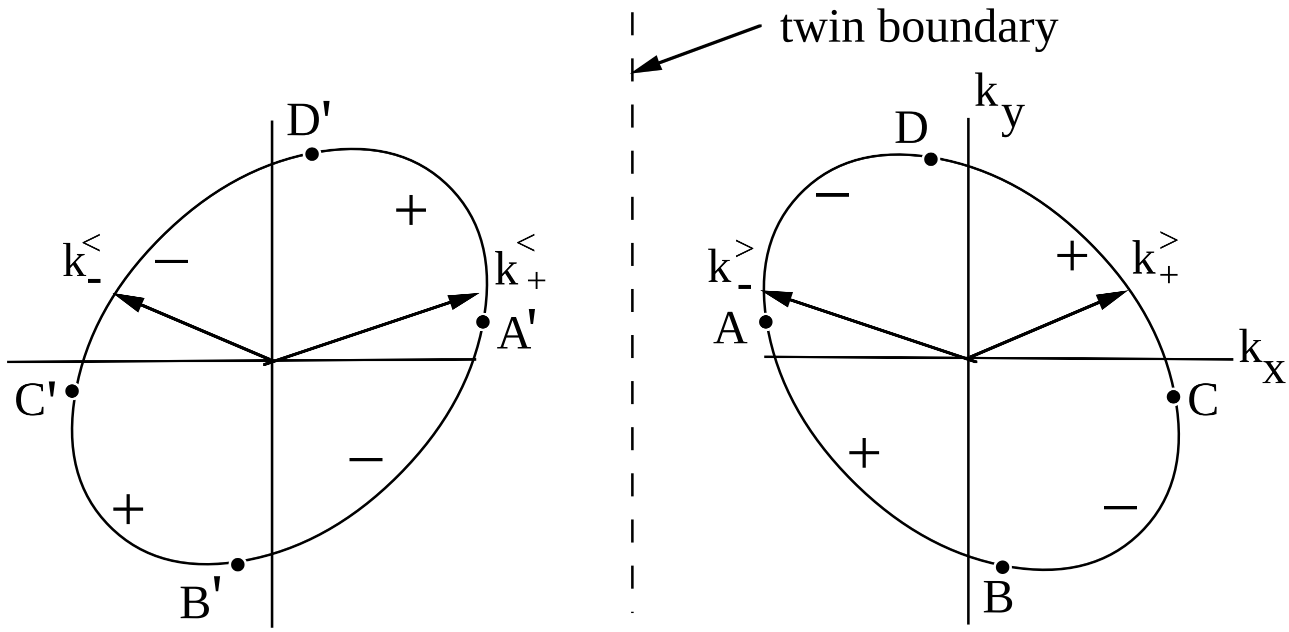
FIG. 1. Twin boundary and nearest-neighbor hopping and pairing amplitudes; $1 \equiv (t_1, \Delta_1/2)$, $\bar{1} \equiv (t_1, -\Delta_1/2)$, $1' \equiv (t_1, \Delta_1'/2)$, $\bar{1}' \equiv (t_1, -\Delta_1'/2)$, $2 \equiv (t_2, -\Delta_2/2)$ etc.

FIG. 2. Twin boundary and orthorhombic Fermi surfaces in the two twins. The capital letters A, B, ... denote the positions of nodes of the $d \pm s$ gaps. The sign of $\Delta(\mathbf{k})$ in the different regions on the Fermi surfaces is indicated as + or −.


y
twin boundary
$\bar{1}$
2'
$\bar{2}'$
1
$\bar{2}$
2
$\bar{1}'$
1'
$\bar{2}$
1
$\bar{1}$
2'
$\bar{2}'$
1
$\bar{2}$
x


twin boundary
D'
A'
B'
C'
D
A
B
C
$k_-^<$
$k_+^<$
$k_-^>$
$k_+^>$
k_y
k_x
+
−
+
−
−
+
+
−